



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:12 PM GMT

PDB ID : 1NWR  
Title : Crystal structure of human cartilage gp39 (HC-gp39)  
Authors : Fusetti, F.; Pijning, T.; Kalk, K.H.; Bos, E.; Dijkstra, B.W.  
Deposited on : 2003-02-06  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

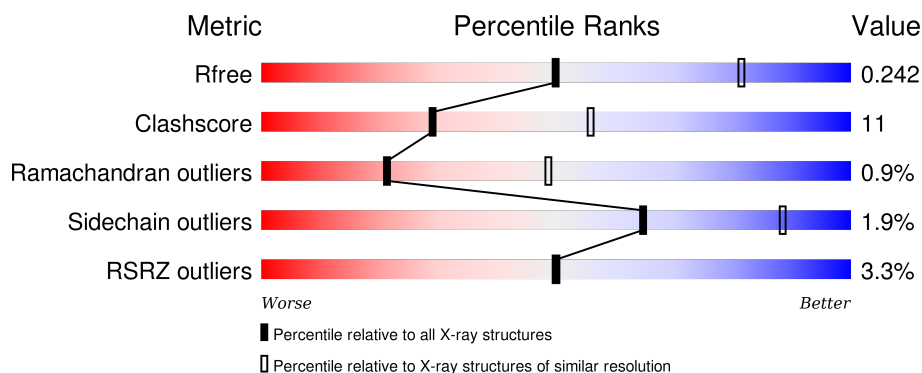
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	362	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	362	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
1	C	362	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
1	D	362	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>26%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11651 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chitinase-3 like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2857	1825	492	529	11			
1	B	362	Total	C	N	O	S	0	0	0
			2857	1825	492	529	11			
1	C	362	Total	C	N	O	S	0	0	0
			2857	1825	492	529	11			
1	D	362	Total	C	N	O	S	0	0	0
			2857	1825	492	529	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	CONFLICT	UNP P36222
B	311	ILE	THR	CONFLICT	UNP P36222
C	311	ILE	THR	CONFLICT	UNP P36222
D	311	ILE	THR	CONFLICT	UNP P36222

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

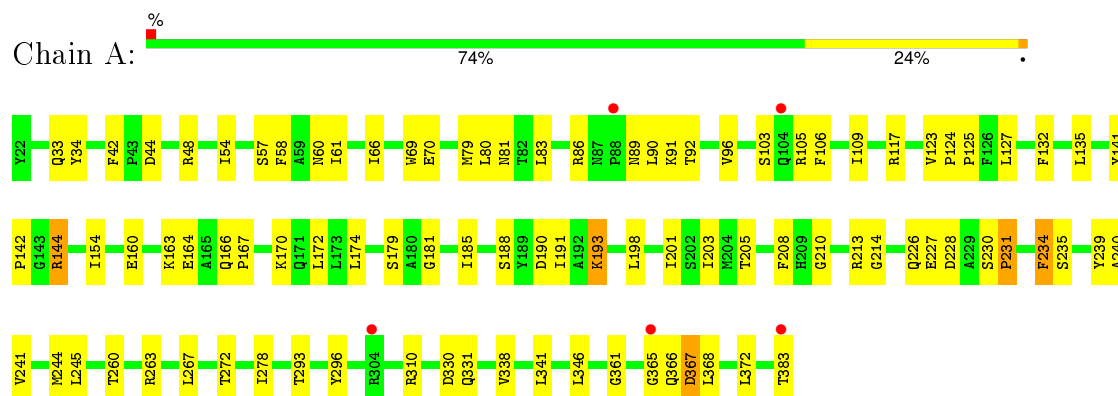
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	16	Total 16	O 16	0	0
3	C	28	Total 28	O 28	0	0
3	D	29	Total 29	O 29	0	0

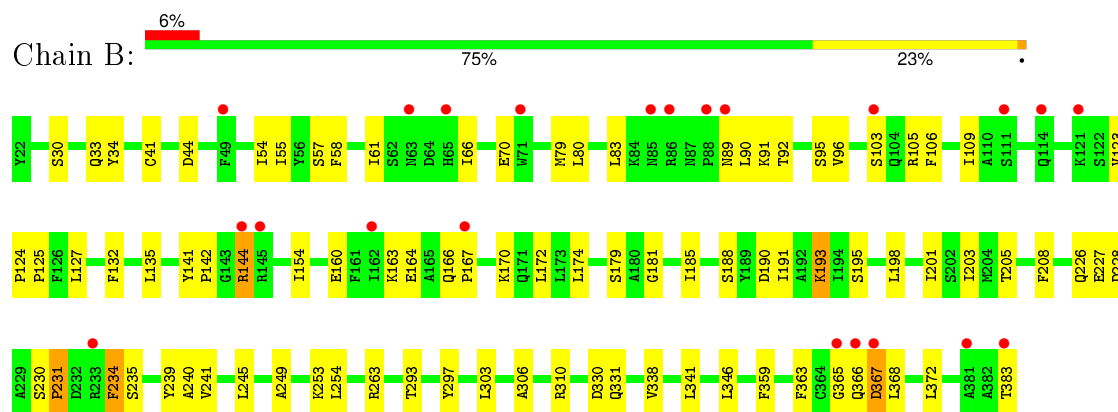
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

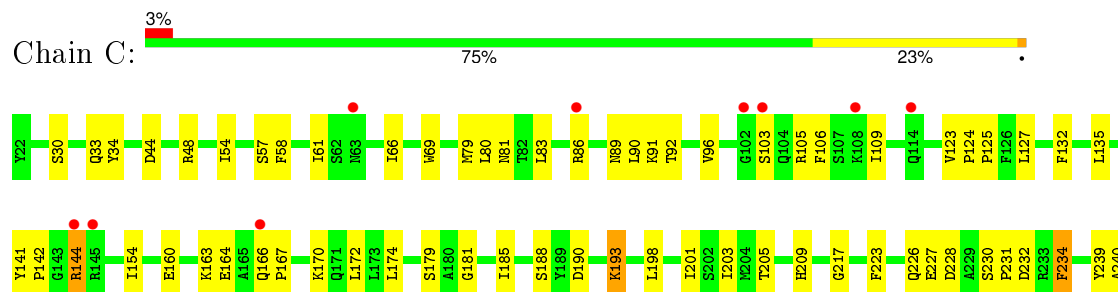
#### • Molecule 1: Chitinase-3 like protein 1



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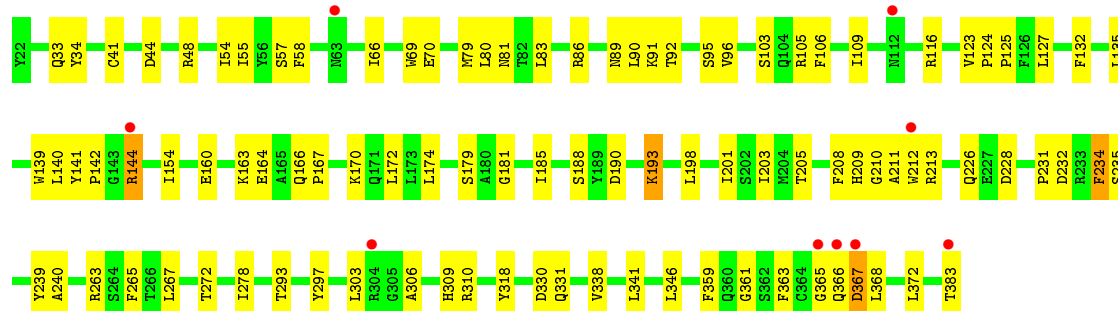
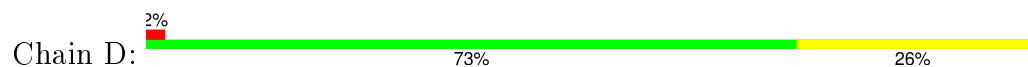


#### • Molecule 1: Chitinase-3 like protein 1





● Molecule 1: Chitinase-3 like protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.30Å 127.30Å 107.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.70 19.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.8 (19.79-2.70) 82.9 (19.79-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.239 0.217 , 0.242	Depositor DCC
$R_{free}$ test set	5574 reflections (14.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.8	EDS
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 39074 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.3595e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/2933	0.61	0/3973
1	B	0.38	0/2933	0.60	0/3973
1	C	0.41	0/2933	0.61	0/3973
1	D	0.42	0/2933	0.62	0/3973
All	All	0.41	0/11732	0.61	0/15892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2857	0	2775	58	0
1	B	2857	0	2775	60	0
1	C	2857	0	2775	65	0
1	D	2857	0	2775	72	0
2	A	28	0	25	5	0
2	B	28	0	25	1	0
2	C	28	0	25	2	0
2	D	28	0	25	2	0
3	A	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	0	0	0
3	C	28	0	0	4	0
3	D	29	0	0	3	0
All	All	11651	0	11200	260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLN:HE21	1:C:228:ASP:HB2	1.42	0.82
1:B:234:PHE:HB3	1:B:239:TYR:CD2	2.15	0.81
2:A:411:NAG:H61	2:A:412:NAG:H82	1.63	0.81
1:D:234:PHE:HB3	1:D:239:TYR:CD2	2.16	0.80
1:C:234:PHE:HB3	1:C:239:TYR:CD2	2.16	0.80
1:B:92:THR:HG22	1:B:132:PHE:HD1	1.46	0.80
1:D:226:GLN:HE21	1:D:228:ASP:HB2	1.48	0.79
1:D:92:THR:HG22	1:D:132:PHE:HD1	1.49	0.77
1:A:92:THR:HG22	1:A:132:PHE:HD1	1.48	0.77
1:C:92:THR:HG22	1:C:132:PHE:HD1	1.49	0.75
1:A:226:GLN:HE21	1:A:228:ASP:HB2	1.53	0.72
1:B:92:THR:HG22	1:B:132:PHE:CD1	2.27	0.70
1:C:92:THR:HG22	1:C:132:PHE:CD1	2.28	0.68
1:D:92:THR:HG22	1:D:132:PHE:CD1	2.28	0.68
1:D:210:GLY:O	1:D:213:ARG:HG3	1.94	0.68
2:A:411:NAG:H61	2:A:412:NAG:C7	2.24	0.67
2:A:411:NAG:H61	2:A:412:NAG:C8	2.25	0.66
1:A:92:THR:HG22	1:A:132:PHE:CD1	2.28	0.66
1:A:234:PHE:HB3	1:A:239:TYR:CD2	2.32	0.65
1:A:203:ILE:HD11	1:A:240:ALA:HB1	1.78	0.64
2:A:411:NAG:C6	2:A:412:NAG:H82	2.26	0.64
1:C:341:LEU:HB2	1:C:346:LEU:HD12	1.81	0.63
1:B:341:LEU:HB2	1:B:346:LEU:HD12	1.80	0.63
1:D:341:LEU:HB2	1:D:346:LEU:HD12	1.82	0.62
1:D:54:ILE:HD11	3:D:455:HOH:O	2.00	0.62
1:A:341:LEU:HB2	1:A:346:LEU:HD12	1.80	0.62
2:D:441:NAG:H62	2:D:442:NAG:C7	2.30	0.61
1:C:338:VAL:O	1:C:341:LEU:HG	2.00	0.61
1:C:234:PHE:HB3	1:C:239:TYR:CE2	2.35	0.60
1:B:44:ASP:HB3	1:B:79:MET:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HG12	1:A:205:THR:HG23	1.83	0.59
1:B:203:ILE:HG12	1:B:205:THR:HG23	1.84	0.59
1:B:234:PHE:HB3	1:B:239:TYR:CE2	2.37	0.59
1:B:338:VAL:O	1:B:341:LEU:HG	2.03	0.59
1:D:44:ASP:HB3	1:D:79:MET:HG2	1.84	0.59
1:D:338:VAL:O	1:D:341:LEU:HG	2.03	0.58
1:A:44:ASP:HB3	1:A:79:MET:HG2	1.85	0.58
1:C:310:ARG:NH2	1:C:330:ASP:OD2	2.36	0.58
1:C:86:ARG:HD3	3:C:460:HOH:O	2.02	0.58
1:C:123:VAL:HB	1:C:124:PRO:HD3	1.85	0.58
1:C:124:PRO:HB2	1:C:125:PRO:HD3	1.86	0.58
1:D:124:PRO:HB2	1:D:125:PRO:HD3	1.86	0.58
1:C:198:LEU:HD13	1:C:201:ILE:CG2	2.34	0.58
1:A:198:LEU:HD13	1:A:201:ILE:CG2	2.34	0.58
1:A:310:ARG:NH2	1:A:330:ASP:OD2	2.36	0.57
1:B:310:ARG:NH2	1:B:330:ASP:OD2	2.38	0.57
1:B:166:GLN:N	1:B:167:PRO:HD2	2.20	0.57
1:D:44:ASP:HB3	1:D:79:MET:CG	2.35	0.57
1:C:44:ASP:HB3	1:C:79:MET:HG2	1.86	0.57
1:A:166:GLN:N	1:A:167:PRO:HD2	2.20	0.56
1:C:44:ASP:HB3	1:C:79:MET:CG	2.36	0.56
1:B:127:LEU:HD12	1:B:172:LEU:HD13	1.87	0.56
1:D:166:GLN:N	1:D:167:PRO:HD2	2.21	0.56
1:D:198:LEU:HD13	1:D:201:ILE:CG2	2.36	0.56
1:A:124:PRO:HB3	1:A:164:GLU:HG3	1.87	0.56
1:B:44:ASP:HB3	1:B:79:MET:CG	2.35	0.56
1:A:338:VAL:O	1:A:341:LEU:HG	2.06	0.56
1:C:166:GLN:N	1:C:167:PRO:HD2	2.21	0.56
1:B:123:VAL:HB	1:B:124:PRO:HD3	1.88	0.56
1:B:198:LEU:HD13	1:B:201:ILE:CG2	2.36	0.56
1:D:123:VAL:HB	1:D:124:PRO:HD3	1.88	0.55
1:D:203:ILE:HG12	1:D:205:THR:HG23	1.89	0.55
1:C:127:LEU:HD12	1:C:172:LEU:HD13	1.87	0.55
1:C:203:ILE:HG12	1:C:205:THR:HG23	1.88	0.55
1:A:127:LEU:HD12	1:A:172:LEU:HD13	1.89	0.55
1:D:141:TYR:CE2	1:D:179:SER:HB2	2.42	0.55
1:D:69:TRP:CE2	2:D:441:NAG:H82	2.42	0.54
1:D:310:ARG:NH2	1:D:330:ASP:OD2	2.40	0.54
1:D:127:LEU:HD12	1:D:172:LEU:HD13	1.88	0.54
1:A:141:TYR:CE2	1:A:179:SER:HB2	2.42	0.54
1:A:124:PRO:HB2	1:A:125:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:VAL:O	1:C:245:LEU:HG	2.08	0.54
1:D:124:PRO:HB3	1:D:164:GLU:HG3	1.88	0.54
1:B:124:PRO:HB2	1:B:125:PRO:HD3	1.90	0.54
1:B:54:ILE:HG13	1:B:90:LEU:HD11	1.89	0.54
1:A:44:ASP:HB3	1:A:79:MET:CG	2.37	0.54
1:B:105:ARG:O	1:B:109:ILE:HG13	2.07	0.54
1:B:141:TYR:CE2	1:B:179:SER:HB2	2.42	0.53
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.89	0.53
1:C:198:LEU:HD13	1:C:201:ILE:HG22	1.90	0.53
1:B:124:PRO:HB3	1:B:164:GLU:HG3	1.89	0.53
1:A:66:ILE:O	1:A:66:ILE:HG23	2.08	0.53
1:C:105:ARG:O	1:C:109:ILE:HG13	2.09	0.53
1:A:69:TRP:CE2	2:A:411:NAG:H82	2.43	0.53
1:D:234:PHE:HB3	1:D:239:TYR:CE2	2.43	0.53
1:D:105:ARG:O	1:D:109:ILE:HG13	2.08	0.52
1:B:198:LEU:O	1:B:253:LYS:NZ	2.32	0.52
1:C:54:ILE:HG13	1:C:90:LEU:HD11	1.91	0.52
1:D:211:ALA:HA	1:D:265:PHE:CE1	2.45	0.52
1:D:198:LEU:HD13	1:D:201:ILE:HG22	1.92	0.52
1:A:105:ARG:O	1:A:109:ILE:HG13	2.09	0.52
1:A:198:LEU:HD13	1:A:201:ILE:HG22	1.91	0.52
1:D:209:HIS:CE1	1:D:213:ARG:HD3	2.45	0.51
1:D:66:ILE:HG23	1:D:66:ILE:O	2.10	0.51
1:A:170:LYS:HG3	1:A:170:LYS:O	2.11	0.51
1:D:54:ILE:HG13	1:D:90:LEU:HD11	1.93	0.51
1:B:198:LEU:HD13	1:B:201:ILE:HG22	1.92	0.51
1:B:80:LEU:HD12	1:B:83:LEU:HD12	1.92	0.51
1:B:66:ILE:O	1:B:66:ILE:HG23	2.10	0.51
1:D:210:GLY:HA3	1:D:212:TRP:CD1	2.46	0.50
1:C:170:LYS:HG3	1:C:170:LYS:O	2.11	0.50
1:B:154:ILE:HD13	1:B:198:LEU:HD11	1.94	0.50
1:C:141:TYR:CE2	1:C:179:SER:HB2	2.46	0.50
1:C:230:SER:HB3	3:C:441:HOH:O	2.10	0.50
1:A:203:ILE:HD12	1:A:244:MET:SD	2.52	0.50
1:B:41:CYS:HB2	1:B:359:PHE:CZ	2.46	0.50
1:B:226:GLN:HE21	1:B:228:ASP:HB2	1.75	0.50
1:B:170:LYS:O	1:B:170:LYS:HG3	2.12	0.50
1:B:208:PHE:HB3	1:B:235:SER:HB3	1.94	0.50
1:C:124:PRO:HB3	1:C:164:GLU:HG3	1.92	0.50
1:B:33:GLN:HG3	1:B:34:TYR:CD1	2.47	0.50
1:D:203:ILE:HD11	1:D:240:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:TRP:CE2	2:C:431:NAG:H82	2.47	0.49
1:A:263:ARG:NH1	1:A:293:THR:OG1	2.45	0.49
1:A:54:ILE:HG13	1:A:90:LEU:HD11	1.95	0.49
1:C:80:LEU:HD12	1:C:83:LEU:HD12	1.94	0.49
1:C:86:ARG:NH1	3:C:460:HOH:O	2.45	0.48
1:A:234:PHE:HB3	1:A:239:TYR:CE2	2.47	0.48
1:A:154:ILE:HD13	1:A:198:LEU:HD11	1.95	0.48
1:A:208:PHE:HB3	1:A:235:SER:HB3	1.94	0.48
1:D:154:ILE:HD13	1:D:198:LEU:HD11	1.94	0.48
1:C:154:ILE:HD13	1:C:198:LEU:HD11	1.95	0.48
1:A:33:GLN:HG3	1:A:34:TYR:CD1	2.48	0.48
1:B:142:PRO:HB2	1:B:188:SER:HB3	1.96	0.48
1:C:263:ARG:NH1	1:C:293:THR:OG1	2.46	0.48
1:C:209:HIS:CD2	1:C:217:GLY:HA3	2.49	0.48
1:A:80:LEU:HD12	1:A:83:LEU:HD12	1.96	0.48
1:C:174:LEU:HG	1:C:198:LEU:HD23	1.96	0.48
1:C:203:ILE:HD11	1:C:240:ALA:HB1	1.96	0.48
1:A:190:ASP:OD1	1:A:193:LYS:HE3	2.14	0.48
1:C:33:GLN:HG3	1:C:34:TYR:CD1	2.48	0.48
1:B:365:GLY:C	1:B:367:ASP:H	2.17	0.47
1:C:66:ILE:HG23	1:C:66:ILE:O	2.13	0.47
1:D:365:GLY:C	1:D:367:ASP:H	2.17	0.47
1:A:210:GLY:O	1:A:213:ARG:HG3	2.14	0.47
1:B:191:ILE:CG2	1:B:249:ALA:HB2	2.44	0.47
1:B:105:ARG:NH1	2:B:421:NAG:H62	2.29	0.47
1:D:170:LYS:O	1:D:170:LYS:HG3	2.13	0.47
1:A:241:VAL:O	1:A:245:LEU:HG	2.14	0.47
1:D:144:ARG:HB3	1:D:144:ARG:NH1	2.29	0.47
1:A:365:GLY:C	1:A:367:ASP:H	2.17	0.47
1:D:211:ALA:HB2	3:D:452:HOH:O	2.14	0.47
1:C:365:GLY:C	1:C:367:ASP:H	2.18	0.47
1:D:142:PRO:HB2	1:D:188:SER:HB3	1.97	0.47
1:D:33:GLN:HG3	1:D:34:TYR:CD1	2.50	0.47
1:B:263:ARG:NH1	1:B:293:THR:OG1	2.48	0.47
1:B:181:GLY:O	1:B:185:ILE:HG13	2.14	0.47
1:C:144:ARG:NH1	1:C:144:ARG:HB3	2.30	0.47
1:D:80:LEU:HD12	1:D:83:LEU:HD12	1.96	0.47
1:D:211:ALA:HA	1:D:265:PHE:HE1	1.80	0.46
1:B:190:ASP:OD1	1:B:193:LYS:HE3	2.16	0.46
1:C:142:PRO:HB2	1:C:188:SER:HB3	1.97	0.46
1:B:174:LEU:HG	1:B:198:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:O	1:B:91:LYS:HD3	2.16	0.46
1:C:190:ASP:OD1	1:C:193:LYS:HE3	2.16	0.46
1:C:57:SER:HA	1:C:58:PHE:HA	1.65	0.45
1:A:174:LEU:HG	1:A:198:LEU:HD23	1.98	0.45
1:D:263:ARG:NH1	1:D:293:THR:OG1	2.49	0.45
1:C:181:GLY:O	1:C:185:ILE:HG13	2.16	0.45
1:A:383:THR:O	1:A:383:THR:HG22	2.17	0.45
1:D:57:SER:HA	1:D:58:PHE:HA	1.67	0.45
1:D:96:VAL:HG12	1:D:135:LEU:HD11	1.97	0.45
1:B:144:ARG:NH1	1:B:144:ARG:HB3	2.32	0.45
1:C:232:ASP:HB3	1:C:234:PHE:H	1.80	0.45
1:C:383:THR:O	1:C:383:THR:HG22	2.17	0.45
1:A:181:GLY:O	1:A:185:ILE:HG13	2.17	0.45
1:B:383:THR:HG22	1:B:383:THR:O	2.17	0.44
1:D:190:ASP:OD1	1:D:193:LYS:HE3	2.16	0.44
1:C:96:VAL:HG12	1:C:135:LEU:HD11	1.99	0.44
1:D:174:LEU:HG	1:D:198:LEU:HD23	1.98	0.44
1:D:303:LEU:HA	1:D:306:ALA:HB3	1.99	0.44
1:C:81:ASN:OD1	1:C:92:THR:HG21	2.17	0.44
1:B:61:ILE:HG21	1:B:109:ILE:HD13	1.99	0.44
1:C:201:ILE:HG13	1:C:254:LEU:HD12	1.99	0.44
1:B:201:ILE:HG13	1:B:254:LEU:HD12	1.99	0.44
1:C:69:TRP:CD2	2:C:431:NAG:H82	2.53	0.44
1:D:34:TYR:HE2	1:D:70:GLU:OE2	2.01	0.44
1:C:366:GLN:O	1:C:368:LEU:N	2.51	0.44
1:A:96:VAL:HG12	1:A:135:LEU:HD11	1.98	0.44
1:B:366:GLN:O	1:B:368:LEU:N	2.51	0.44
1:D:208:PHE:HB3	1:D:235:SER:HB3	2.00	0.43
1:A:160:GLU:OE1	1:A:163:LYS:HD3	2.18	0.43
1:B:366:GLN:C	1:B:368:LEU:H	2.22	0.43
1:A:57:SER:HA	1:A:58:PHE:HA	1.67	0.43
1:A:117:ARG:HB2	3:A:416:HOH:O	2.18	0.43
1:A:144:ARG:HB3	1:A:144:ARG:NH1	2.32	0.43
1:D:383:THR:O	1:D:383:THR:HG22	2.18	0.43
1:A:214:GLY:C	1:A:278:ILE:HG12	2.39	0.43
1:B:96:VAL:HG12	1:B:135:LEU:HD11	1.99	0.43
1:A:260:THR:O	1:A:296:TYR:HB2	2.19	0.43
1:A:89:ASN:O	1:A:91:LYS:HD3	2.19	0.43
1:B:241:VAL:O	1:B:245:LEU:HG	2.18	0.43
1:D:211:ALA:O	1:D:278:ILE:HD11	2.19	0.43
1:C:366:GLN:C	1:C:368:LEU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASP:HA	1:D:372:LEU:HD21	2.00	0.43
1:C:366:GLN:C	1:C:368:LEU:H	2.22	0.43
1:C:160:GLU:OE1	1:C:163:LYS:HD3	2.18	0.43
1:D:366:GLN:O	1:D:368:LEU:N	2.52	0.43
1:D:267:LEU:HD13	1:D:272:THR:HG22	2.01	0.43
1:A:330:ASP:HA	1:A:372:LEU:HD21	2.00	0.42
1:D:55:ILE:CG2	1:D:95:SER:HB2	2.49	0.42
1:C:89:ASN:O	1:C:91:LYS:HD3	2.19	0.42
1:D:89:ASN:O	1:D:91:LYS:HD3	2.19	0.42
1:D:361:GLY:O	1:D:367:ASP:HA	2.20	0.42
1:D:181:GLY:O	1:D:185:ILE:HG13	2.19	0.42
1:D:209:HIS:ND1	1:D:213:ARG:HD3	2.34	0.42
1:D:365:GLY:C	1:D:367:ASP:N	2.73	0.42
1:D:160:GLU:OE1	1:D:163:LYS:HD3	2.20	0.42
1:D:81:ASN:OD1	1:D:92:THR:HG21	2.20	0.42
1:A:34:TYR:HE2	1:A:70:GLU:OE2	2.02	0.42
1:B:366:GLN:C	1:B:368:LEU:N	2.72	0.42
1:D:48:ARG:CZ	1:D:86:ARG:HD2	2.50	0.42
1:C:303:LEU:HA	1:C:306:ALA:HB3	2.02	0.42
1:B:203:ILE:HD11	1:B:240:ALA:HB1	2.01	0.42
1:D:48:ARG:NE	1:D:86:ARG:HB2	2.35	0.42
1:A:81:ASN:OD1	1:A:92:THR:HG21	2.20	0.42
1:B:330:ASP:HA	1:B:372:LEU:HD21	2.02	0.42
1:A:230:SER:HA	1:A:231:PRO:HD3	1.84	0.42
1:A:142:PRO:HB2	1:A:188:SER:HB3	2.02	0.41
1:C:267:LEU:HD13	1:C:272:THR:HG22	2.02	0.41
1:B:57:SER:HA	1:B:58:PHE:HA	1.65	0.41
1:B:297:TYR:HB2	1:B:363:PHE:CG	2.55	0.41
1:D:116:ARG:NH2	3:D:467:HOH:O	2.52	0.41
1:B:303:LEU:HA	1:B:306:ALA:HB3	2.00	0.41
1:D:297:TYR:HB2	1:D:363:PHE:CG	2.55	0.41
1:D:232:ASP:HB3	1:D:234:PHE:H	1.85	0.41
1:B:195:SER:O	1:B:253:LYS:HD3	2.21	0.41
1:B:263:ARG:HA	1:B:263:ARG:HD3	1.94	0.41
1:A:48:ARG:NE	1:A:86:ARG:HB2	2.35	0.41
1:B:230:SER:HA	1:B:231:PRO:HD3	1.85	0.41
1:A:33:GLN:HB2	1:A:42:PHE:CZ	2.55	0.41
1:D:366:GLN:C	1:D:368:LEU:N	2.74	0.41
1:B:160:GLU:OE1	1:B:163:LYS:HD3	2.20	0.41
1:C:30:SER:O	1:C:33:GLN:HG2	2.20	0.41
1:C:330:ASP:HA	1:C:372:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HG2	1:C:86:ARG:NH1	2.36	0.41
1:D:140:LEU:HA	1:D:141:TYR:HA	1.80	0.41
1:C:61:ILE:HG21	1:C:109:ILE:HD13	2.02	0.41
1:B:365:GLY:C	1:B:367:ASP:N	2.74	0.41
1:A:361:GLY:O	1:A:367:ASP:HA	2.21	0.41
1:D:86:ARG:HG2	1:D:86:ARG:NH1	2.36	0.41
1:C:297:TYR:HB2	1:C:363:PHE:CG	2.56	0.41
1:C:341:LEU:CB	1:C:346:LEU:HD12	2.51	0.41
1:D:34:TYR:CE2	1:D:70:GLU:OE2	2.74	0.41
1:D:366:GLN:C	1:D:368:LEU:H	2.23	0.41
1:C:331:GLN:NE2	3:C:454:HOH:O	2.46	0.41
1:A:267:LEU:HD13	1:A:272:THR:HG22	2.03	0.41
1:B:30:SER:O	1:B:33:GLN:HG2	2.21	0.40
1:B:34:TYR:HE2	1:B:70:GLU:OE2	2.03	0.40
1:A:366:GLN:O	1:A:368:LEU:N	2.54	0.40
1:A:366:GLN:C	1:A:368:LEU:N	2.74	0.40
1:D:41:CYS:HB2	1:D:359:PHE:CZ	2.57	0.40
1:C:263:ARG:HA	1:C:263:ARG:HD3	1.93	0.40
1:B:55:ILE:CG2	1:B:95:SER:HB2	2.51	0.40
1:C:48:ARG:CZ	1:C:86:ARG:HD2	2.52	0.40
1:D:139:TRP:O	1:D:141:TYR:HA	2.21	0.40
1:C:365:GLY:C	1:C:367:ASP:N	2.74	0.40
1:A:60:ASN:CG	1:A:61:ILE:H	2.25	0.40
1:C:223:PHE:HB2	1:C:313:GLY:O	2.21	0.40
1:D:309:HIS:HB2	1:D:318:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	360/362 (99%)	339 (94%)	17 (5%)	4 (1%)	17 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	B	360/362 (99%)	338 (94%)	19 (5%)	3 (1%)	24	51	
1	C	360/362 (99%)	339 (94%)	18 (5%)	3 (1%)	24	51	
1	D	360/362 (99%)	341 (95%)	16 (4%)	3 (1%)	24	51	
All	All	1440/1448 (99%)	1357 (94%)	70 (5%)	13 (1%)	21	49	

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	PRO
1	D	231	PRO
1	A	231	PRO
1	B	367	ASP
1	C	367	ASP
1	D	367	ASP
1	A	367	ASP
1	B	231	PRO
1	C	103	SER
1	D	103	SER
1	A	103	SER
1	B	103	SER
1	A	191	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/302 (100%)	295 (98%)	6 (2%)	63	87
1	B	301/302 (100%)	295 (98%)	6 (2%)	63	87
1	C	301/302 (100%)	295 (98%)	6 (2%)	63	87
1	D	301/302 (100%)	296 (98%)	5 (2%)	68	90
All	All	1204/1208 (100%)	1181 (98%)	23 (2%)	65	88

All (23) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	106	PHE
1	A	144	ARG
1	A	193	LYS
1	A	227	GLU
1	A	234	PHE
1	A	331	GLN
1	B	106	PHE
1	B	144	ARG
1	B	193	LYS
1	B	227	GLU
1	B	234	PHE
1	B	331	GLN
1	C	106	PHE
1	C	144	ARG
1	C	193	LYS
1	C	227	GLU
1	C	234	PHE
1	C	331	GLN
1	D	106	PHE
1	D	144	ARG
1	D	193	LYS
1	D	234	PHE
1	D	331	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	226	GLN
1	A	331	GLN
1	A	345	GLN
1	A	366	GLN
1	B	100	ASN
1	B	226	GLN
1	B	331	GLN
1	B	345	GLN
1	B	366	GLN
1	C	100	ASN
1	C	226	GLN
1	C	331	GLN
1	C	345	GLN
1	C	366	GLN
1	D	100	ASN

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Mol	Chain	Res	Type
1	D	226	GLN
1	D	331	GLN
1	D	345	GLN
1	D	366	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	411	1,2	14,14,15	0.68	0	15,19,21	0.94	1 (6%)
2	NAG	A	412	2	14,14,15	0.76	0	15,19,21	0.97	1 (6%)
2	NAG	B	421	1,2	14,14,15	0.56	0	15,19,21	0.73	1 (6%)
2	NAG	B	422	2	14,14,15	0.67	0	15,19,21	0.81	1 (6%)
2	NAG	C	431	1,2	14,14,15	0.54	0	15,19,21	0.80	1 (6%)
2	NAG	C	432	2	14,14,15	0.56	0	15,19,21	0.64	0
2	NAG	D	441	1,2	14,14,15	0.69	0	15,19,21	0.74	0
2	NAG	D	442	2	14,14,15	0.75	0	15,19,21	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	411	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	412	2	-	0/6/23/26	0/1/1/1
2	NAG	B	421	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	422	2	-	0/6/23/26	0/1/1/1
2	NAG	C	431	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	432	2	-	0/6/23/26	0/1/1/1
2	NAG	D	441	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	442	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	NAG	C2-N2-C7	-3.11	119.05	123.04
2	A	412	NAG	C2-N2-C7	-2.59	119.72	123.04
2	C	431	NAG	C2-N2-C7	-2.52	119.80	123.04
2	B	421	NAG	C2-N2-C7	-2.19	120.23	123.04
2	B	422	NAG	C2-N2-C7	-2.06	120.39	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	NAG	5	0
2	A	412	NAG	4	0
2	B	421	NAG	1	0
2	C	431	NAG	2	0
2	D	441	NAG	2	0
2	D	442	NAG	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	362/362 (100%)	-0.33	5 (1%) 78 77	6, 28, 56, 78	0
1	B	362/362 (100%)	0.29	22 (6%) 25 23	14, 49, 82, 87	0
1	C	362/362 (100%)	-0.26	12 (3%) 50 50	5, 30, 65, 82	0
1	D	362/362 (100%)	-0.21	9 (2%) 61 61	6, 28, 56, 78	0
All	All	1448/1448 (100%)	-0.13	48 (3%) 50 50	5, 32, 71, 87	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	THR	4.6
1	C	365	GLY	4.5
1	B	366	GLN	3.8
1	B	89	ASN	3.7
1	A	383	THR	3.6
1	B	63	ASN	3.6
1	B	103	SER	3.5
1	B	162	ILE	3.3
1	A	304	ARG	3.1
1	B	367	ASP	3.1
1	C	145	ARG	3.0
1	B	365	GLY	2.9
1	D	367	ASP	2.9
1	D	63	ASN	2.9
1	B	49	PHE	2.9
1	B	114	GLN	2.8
1	C	366	GLN	2.8
1	B	144	ARG	2.8
1	B	145	ARG	2.8
1	C	383	THR	2.8
1	B	65	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	304	ARG	2.7
1	C	102	GLY	2.7
1	B	167	PRO	2.7
1	D	383	THR	2.6
1	A	365	GLY	2.5
1	B	85	ASN	2.5
1	B	71	TRP	2.4
1	B	111	SER	2.4
1	C	114	GLN	2.4
1	A	88	PRO	2.3
1	B	233	ARG	2.3
1	D	212	TRP	2.3
1	B	86	ARG	2.3
1	C	103	SER	2.3
1	C	144	ARG	2.2
1	B	121	LYS	2.2
1	C	86	ARG	2.2
1	A	104	GLN	2.2
1	D	366	GLN	2.2
1	C	108	LYS	2.1
1	C	63	ASN	2.1
1	D	112	ASN	2.1
1	B	88	PRO	2.1
1	D	365	GLY	2.1
1	D	144	ARG	2.0
1	B	381	ALA	2.0
1	C	166	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	421	14/15	0.88	0.28	0.46	54,65,72,77	0
2	NAG	C	431	14/15	0.91	0.22	0.42	16,38,59,62	0
2	NAG	A	411	14/15	0.92	0.19	0.38	25,32,47,53	0
2	NAG	D	441	14/15	0.91	0.15	-0.60	27,35,44,56	0
2	NAG	D	442	14/15	0.84	0.35	-	47,58,82,88	0
2	NAG	C	432	14/15	0.81	0.42	-	38,57,71,71	0
2	NAG	B	422	14/15	0.84	0.40	-	56,61,68,70	0
2	NAG	A	412	14/15	0.89	0.29	-	12,42,56,58	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.